> d his

(FILE 'HOME' ENTERED AT 08:46:14 ON 03 MAR 2005)

FILE 'REGISTRY' ENTERED AT 08:46:44 ON 03 MAR 2005
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 2 S L1 FUL
L4 STRUCTURE UPLOADED
L5 0 S L4
L6 12 S L4 FUL

FILE 'REGISTRY' ENTERED AT 08:52:19 ON 03 MAR 2005
L7 0 S L6

FILE 'CAPLUS' ENTERED AT 08:52:28 ON 03 MAR 2005
L8 7 S L6

=> d l4
L4 HAS NO ANSWERS
L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

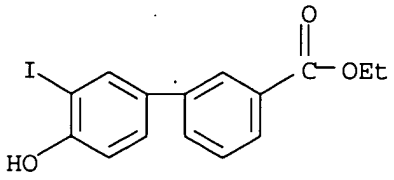
=> d bib abs hitstr 1-7

L8 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:1070486 CAPLUS
DN 142:168979
TI 4-(2-[2-(2(R)-Methylpyrrolidin-1-yl)ethyl]benzofuran-5-yl)benzonitrile and Related 2-Aminoethylbenzofuran H3 Receptor Antagonists Potently Enhance Cognition and Attention
AU Cowart, Marlon; Faghih, Ramin; Curtis, Michael P.; Gfesser, Gregory A.; Bennani, Youssef L.; Black, Lawrence A.; Pan, Liping; Marsh, Kennan C.; Sullivan, James P.; Esbenshade, Timothy A.; Fox, Gerard B.; Hancock, Arthur A.
CS Department of Neuroscience Research and Department of Drug Metabolism and Pharmacokinetics, Abbott Laboratories, Abbott Park, IL, 60064-6123, USA
SO Journal of Medicinal Chemistry (2005), 48(1), 38-55
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB H3 receptor antagonists based on a 2-aminoethylbenzofuran skeleton have been discovered, which are potent in vitro at human and rat H3 receptors, with Ki values of 0.1-5.8 nM. Analogs were discovered with potent (0.01-1 mg/kg) cognition and attention enhancing properties in animal models. One compound in particular, 4-(2-[2-(2(R)-methylpyrrolidin-1-yl)ethyl]benzofuran-5-yl)benzonitrile (ABT-239), combined potent and selective H3 receptor antagonism and excellent pharmacokinetic and metabolic properties across species, with full efficacy in two behavioral models: a five-trial inhibitory avoidance acquisition model in rat pups at 0.1 mg/kg and a social recognition memory model in adult rats at 0.01 mg/kg. Furthermore, this compound did not stimulate locomotor activity and showed high selectivity for the induction of behavioral efficacy vs. central nervous system based side effects. The potency and selectivity of this compound and of analogs from this class support the potential of H3 receptor antagonists for the treatment of cognitive dysfunction.
IT **460748-54-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(4-(2-[2-(2(R)-methylpyrrolidin-1-yl)ethyl]benzofuran-5-yl)benzonitrile and related 2-aminoethylbenzofuran H3 receptor antagonists potently enhance cognition and attention)

RN 460748-54-3 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 4'-hydroxy-3'-iodo-, ethyl ester (9CI) (CA INDEX NAME)



RE.CNT 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:736244 CAPLUS

DN 137:247602

TI Preparation of (pyrrolidinylalkyl)benzofurans and analogs as histamine-3 receptor ligands for treatment of disorders related to CNS neurotransmission

IN Cowart, Marlon D.; Bennani, Youssef L.; Faghih, Ramin; Gfesser, Gregory A.; Black, Lawrence A.

PA Abbott Laboratories, USA

SO PCT Int. Appl., 268 pp.
CODEN: PIXXD2

DT Patent

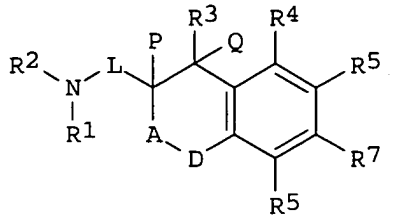
LA English

FAN.CNT 2

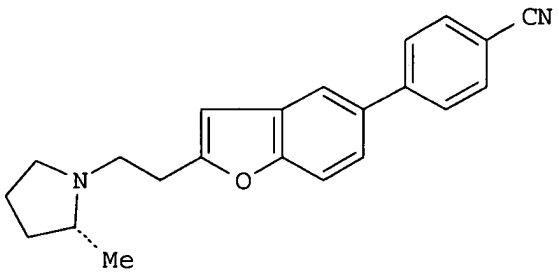
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002074758	A2	20020926	WO 2002-US7107	20020311
	WO 2002074758	A3	20030320		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2002177589	A1	20021128	US 2001-810648	20010316
	US 2002183309	A1	20021205	US 2002-44495	20020111
	US 2002169188	A1	20021114	US 2002-81207	20020225
	CA 2440238	AA	20020926	CA 2002-2440238	20020311
	EP 1370546	A2	20031217	EP 2002-715079	20020311
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2005500986	T2	20050113	JP 2002-573767	20020311
PRAI	US 2001-276793P	P	20010316		
	US 2001-810648	A	20010316		
	US 2002-44495	A	20020111		
	US 2002-81207	A	20020225		
	WO 2002-US7107	W	20020311		

OS MARPAT 137:247602

GI



I



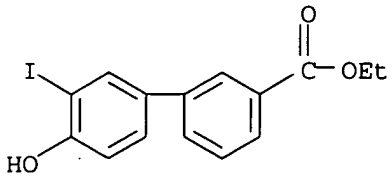
II

AB Title compds. I [wherein A = CO or covalent bond; D = O or S; L = alkylene, fluoroalkylene, or hydroxyalkylene; P and Q taken together form a covalent bond or are both H; R1 and R2 = independently H, (cyclo)alkyl, aryl(alkyl), cycloalkylalkyl, heterocyclyl(alkyl), hydroxyalkyl, alkenyl, or alkynyl; or NR1R2 = heterocyclyl; R3 = H, alkoxy(carbonyl), (halo)alkyl, alkylcarbonyl(oxy), alkylsufinyl, alkylsulfonyl, alkylthio, aryl, carboxy(alkyl), cyano(alkyl), formyl, halo(alkoxy), heterocyclyl, hydroxy(alkyl), SH, NO2, or (un)substituted amino(alkyl), carbamoyl, or sulfamoyl; R4-R7 = independently R3 or L2R20 or R20L3R22; L2 = alkylene, alkenylene, O, S, SO, SO2, CO, C:NOR21, or (un)substituted amino; L3 = covalent bond, alkylene, alkenylene, O, S, CO, N:OR21, or (un)substituted amino; R20 and R22 = independently aryl, heterocyclyl, or cycloalkyl; R21 = H or alkyl; or pharmaceutically acceptable salts, esters, amides, or prodrugs thereof] where prepared for modulation of the histamine-3 (H3) receptors. For example, 4-hydroxy-4'-cyanobiphenyl was treated with NaI, NaOH, and NaOCl in MeOH to give 4'-hydroxy-3'-iodo-[1,1'-biphenyl]-4-carbonitrile (53%). Cyclization with 3-butyn-1-ol in DMF in the presence of CuI and Pd(PPh3)2Cl2 afforded 4-[2-(2-hydroxyethyl)-1-benzofuran-5-yl]benzonitrile (95%). Mesylation (89%), followed by addition of (2R)-2-methylpyrrolidine•HBr and Na2CO3 in AcCN (34%), produced II. The latter displayed binding activity to H3 receptors in rat brain cortex tissue with Ki of 4.44 nM. I are H3 receptor ligands that modulate function of the H3 receptor by antagonizing its activity. Thus, I are useful for the treatment of disorders ameliorated by H3 receptor ligands, especially Alzheimer's disease, attention-deficit hyperactivity disorder, epilepsy, narcolepsy, obesity, cognitive impairment, deficits of memory, deficits of learning, and dementia (no data).

IT **460748-54-3P**, Ethyl 4'-hydroxy-3'-iodo-1,1'-biphenyl-3-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of (pyrrolidinylalkyl)benzofurans and analogs as histamine-3 receptor ligands for treatment of disorders related to CNS neurotransmission)

RN 460748-54-3 CAPLUS

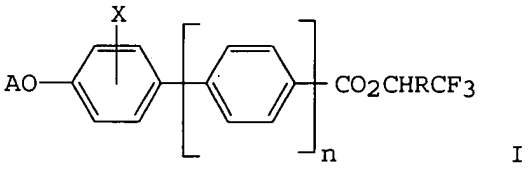
CN [1,1'-Biphenyl]-3-carboxylic acid, 4'-hydroxy-3'-iodo-, ethyl ester (9CI) (CA INDEX NAME)



L8 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:491850 CAPLUS
DN 115:91850
TI Optically active hydroxyarenecarboxylic acid 1-(trifluoromethyl)alkyl esters as intermediates for ferroelectric liquid crystals
IN Ozawa, Tetsuo; Fukahori, Choko
PA Mitsubishi Kasei Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 03058957	A2	19910314	JP 1989-195965	19890728
PRAI	JP 1989-195965		19890728		

OS MARPAT 115:91850
GI

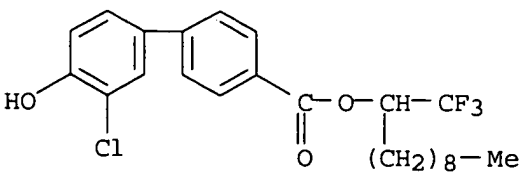


I

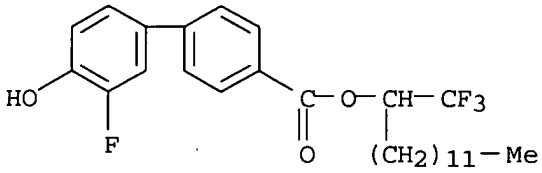
AB The title esters I [A = H; R = C2-18 alkyl, CH2CH2OR1, (CH2)3OR1, CH2CO2R1; R1 = C1-18 alkyl; X = lower alkyl, halo; n = 0, 1] (II) are prepared 3,4-Cl(AcO)C6H3CO2H (1.0 g) was treated with SOCl2 under reflux for 3 h and the resulting acid chloride treated with 0.86 g (-)-Me(CH2)5CH(CF3)OH and triethylenediamine in toluene at 25° for 3 h to give 0.52 g I (A = Ac, R = hexyl, X = 3-Cl, n = 0), 0.5 g of which in (Me2CH)2O was treated with BuNH2 at room temperature for 12 h to give 0.45 g II (R = hexyl, X = 3-Cl, n = 0).

IT **135412-69-0P 135412-70-3P 135412-77-0P**
135412-78-1P 135412-85-0P 135412-86-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for ferroelec. liquid crystals)

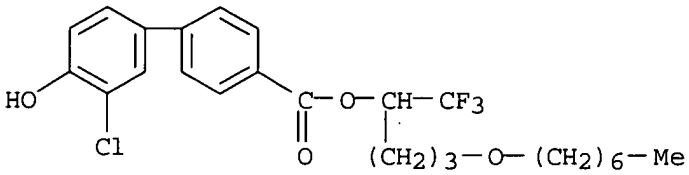
RN 135412-69-0 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-chloro-4'-hydroxy-, 1-(trifluoromethyl)decyl ester (9CI) (CA INDEX NAME)



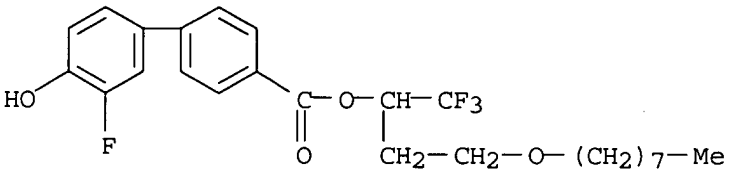
RN 135412-70-3 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 1-(trifluoromethyl)tridecyl ester (9CI) (CA INDEX NAME)



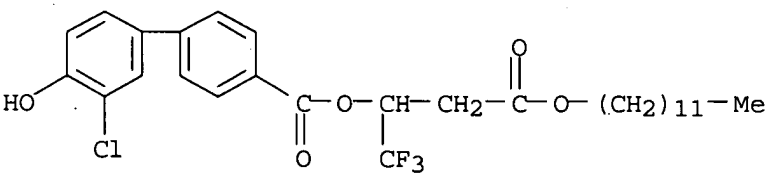
RN 135412-77-0 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-chloro-4'-hydroxy-, 4-(heptyloxy)-1-(trifluoromethyl)butyl ester (9CI) (CA INDEX NAME)



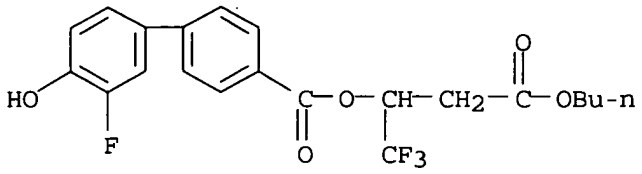
RN 135412-78-1 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 3-(octyloxy)-1-(trifluoromethyl)propyl ester (9CI) (CA INDEX NAME)



RN 135412-85-0 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-chloro-4'-hydroxy-, 3-(dodecyloxy)-3-oxo-1-(trifluoromethyl)propyl ester (9CI) (CA INDEX NAME)



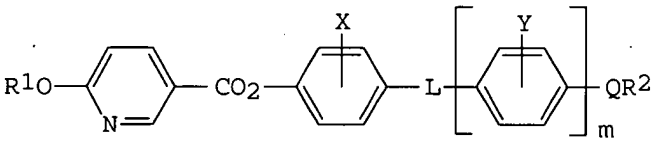
RN 135412-86-1 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 3-butoxy-3-oxo-1-(trifluoromethyl)propyl ester (9CI) (CA INDEX NAME)



L8 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:15021 CAPLUS
DN 114:15021
TI Optically-active 6-alkoxy-3-pyridinecarboxylic acid esters, liquid-crystal compositions containing them, and optical switching devices
IN Sugawara, Shungo
PA Nippon Telegraph and Telephone Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 02056466	A2	19900226	JP 1988-206385	19880822
PRAI	JP 1988-206385		19880822		

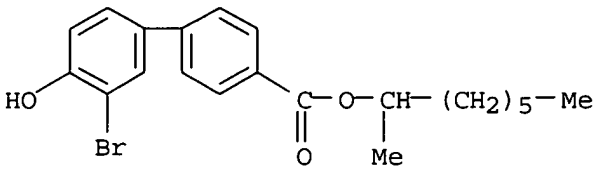
GI



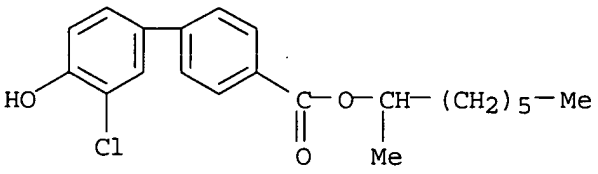
I

AB The title esters I (R1, R2 = C≥4 alkyl; L = CO2, OCO, direct bond; R1 and/or R2 = optically active; Q = CO2, O, direct bond; X, Y = H, halo; X and/or Y = halo; m =0, 1; L = direct bond and Q = CO2, O when m = 0), liquid-crystal compns. containing ≥1 I, and optical switching devices using I or liquid-crystal compns. containing ≥1 I are claimed. I or liquid-crystal compns. containing I have large spontaneous polarization and show chiral smectic phase with wide mesomorphic range, thus permit quick response of display cell. 6-Decyloxynicotinic acid was treated with 3-fluoro-4-hydroxybenzoic acid, 1-methylheptyl 3-fluoro-4-hydroxybenzoate to give I [R1 = decyl, QR2 = CO2CHMe(CH2)5Me, L = CO2, m = 1; X = Y = 2-F] (II) showing a chiral smectic C phase. An optical switching cell packed with II was prepared

IT **128379-21-5P 130976-89-5P**
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of, with alkoxynicotinic acid, chiral smectic C liquid crystal from)
RN 128379-21-5 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-bromo-4'-hydroxy-, 1-methylheptyl ester (9CI) (CA INDEX NAME)



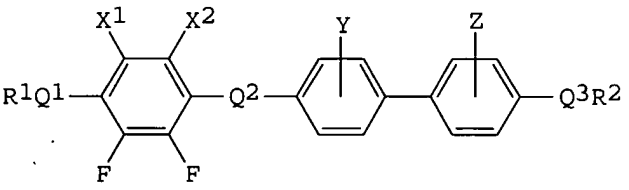
RN 130976-89-5 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-chloro-4'-hydroxy-, 1-methylheptyl ester (9CI) (CA INDEX NAME)



L8 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1990:468511 CAPLUS
DN 113:68511
TI Optically-active biphenyl derivatives, liquid-crystal compositions, and optical switching devices
IN Sugawara, Shungo
PA Nippon Telegraph and Telephone Corp., Japan
SO Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 02059544	A2	19900228	JP 1988-210541	19880826
PRAI JP 1988-210541		19880826		

OS MARPAT 113:68511
GI



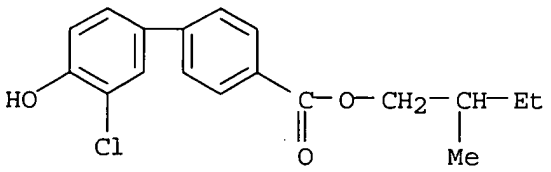
I

AB The title derivs. I (R1, R2 = C≥4 alkyl; X1, X2 = F, Cl; Y and/or Z = halo and the other = H; Q1 = O, OCO; Q2 = CO2, OCO; Q3 = CO2, O; R1 and/or R2 = optically-active), liquid-crystal compns. containing ≥1 I, and optical switching devices using I or liquid-crystal compns. containing ≥1 I are claimed. I or liquid-crystal compns. containing I show a chiral smectic C phase and permit quick response of display devices. 3-Fluoro-4-bromophenol was coupled with 3-fluoro-4-(1-methylheptyloxy)bromobenzene and the resulting biphenyl derivative was treated with 4-decyloxytetrafluorobenzoic acid to give I [Q1R1 = decyloxy, Q3R2 = optically-active OCHMe(CH2)5Me; Q2 = CO2, X1 = X2 = F, Y = 2-F, Z = 3-F] (II), showing a chiral smectic C phase. An optical switching cell packed

with II showed quick response.

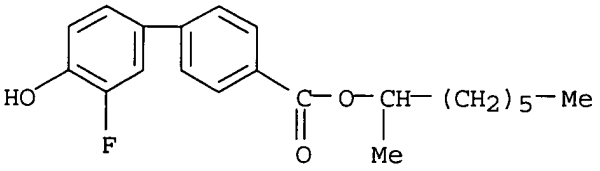
IT **128379-19-1**
RL: USES (Uses)
(Preparation and esterification with, of alkoxytetrahalobenzoic acids, chiral smectic C liquid crystals from)

RN 128379-19-1 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-chloro-4'-hydroxy-, 2-methylbutyl ester (9CI) (CA INDEX NAME)

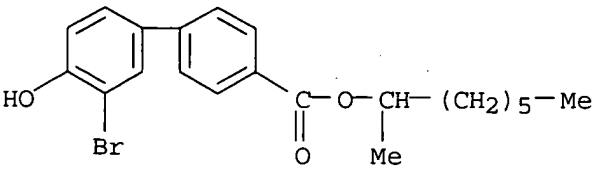


IT **128379-20-4 128379-21-5**
RL: USES (Uses)
(condensation of, with pentahalobenzonitriles, in preparation of chiral smectic C liquid crystals)

RN 128379-20-4 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 1-methylheptyl ester (9CI) (CA INDEX NAME)



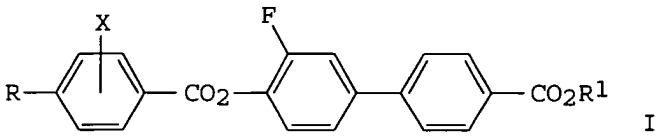
RN 128379-21-5 CAPLUS
CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-bromo-4'-hydroxy-, 1-methylheptyl ester (9CI) (CA INDEX NAME)



L8 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:85399 CAPLUS
DN 108:85399
TI Fluorobiphenyl benzoate derivative liquid crystals for optical switching devices for display
IN Shoji, Tadao; Osawa, Masashi; Takehara, Sadao; Fujisawa, Noburu; Ogawa, Hiroshi
PA Dainippon Ink and Chemicals, Inc., Japan; Kawamura Physical and Chemical Research Institute
SO Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 62181239	A2	19870808	JP 1986-22897	19860206
	JP 07014899	B4	19950222		
PRAI	JP 1986-22897		19860206		

GI



I

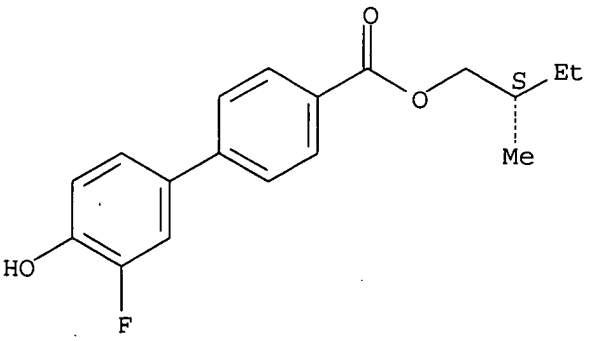
AB The title compds. I (R = C≤20 alkyl, alkoxy; R1 = optically active group; X = H, halo) are useful for optical switching devices. The compds. show ferroelectricity and provide liquid-crystal display devices with rapid response. Thus, 4-C10H21OC6H4CO2H was refluxed with SOCl2 and then treated with (S)-2-methylbutyl 3'-fluoro-4'-hydroxy-4-biphenylcarboxylate at 60-70° for 3 h and let stand overnight to give I [R = C10H21O, R1 = (S)-CH2CHMeEt, X = H] (II). A mixture of II 50 and (S)-2-methylbutyl 4-(3'-fluoro-4'-decyloxybiphenyl-4-carbonyloxy)benzoate (chiral smectic phase at 54.0-124.2°) 50% showed chiral smectic phase at 13.8-146.5° and response time 550 μs at 65° when used in liquid crystal display cell.

IT **106316-31-8P**
RL: PREP (Preparation)
(preparation and esterification of alkoxybenzoic acids with, in liquid-crystal preparation)

RN 106316-31-8 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 2-methylbutyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1987:59023 CAPLUS

DN 106:59023

TI Liquid crystalline compounds having substituents

IN Takehara, Sadao; Fujisawa, Toru; Arai, Yoshi; Kurokawa, Jitsuo

PA Dainippon Ink Chemical Industry Co., Japan; Kawamura Physical and Chemical Research Institute

SO Eur. Pat. Appl., 57 pp.
CODEN: EPXXDW

DT Patent

LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 188222	A2	19860723	EP 1986-100165	19860108
	EP 188222	A3	19861105		
	EP 188222	B1	19920429		
	R: CH, DE, GB, LI				
	JP 61161244	A2	19860721	JP 1985-1791	19850109
	JP 06029222	B4	19940420		
	JP 61229841	A2	19861014	JP 1985-71628	19850404
	JP 06029223	B4	19940420		
	JP 61238762	A2	19861024	JP 1985-81688	19850417
	JP 06029224	B4	19940420		
	JP 61249953	A2	19861107	JP 1985-90676	19850426
	JP 06078280	B4	19941005		
	US 4828754	A	19890509	US 1988-161421	19880223
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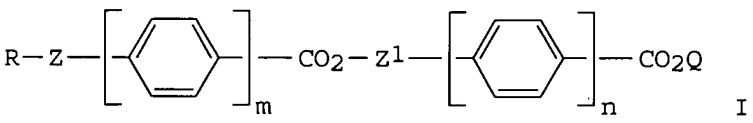
	JP 1985-71628	A	19850404		
	JP 1985-81688	A	19850417		
	JP 1985-90676	A	19850426		
	US 1986-815935	A1	19860103		

OS CASREACT 106:59023
GI



I

AB Liquid crystal compds. for display devices are represented by I, where R is a C1-20 alkyl or alkoxy group; m and n are each 0 or 1, provided m and n are not 1 at the same time; Z is a 2-X-1,4-phenylene or 3-X-1,4-phenylene group and Z1 is a 2-Y-1,4-phenylene or 3-Y-1,4-phenylene group, where X and Y are each H, a halogen atom or a nitro group, provided X and Y are not H at the same time; and Q is an optically active group having a chiral C atom and a linear or cyclic alkyl or alkenyl group which may be substituted by a halogen atom. When Q is a 2-methylbutyl group, a 1-methylalkyl group having 4-8 C atoms, or a 2-chloropropyl group, the liquid crystal compound may have a chiral smectic C phase. Thus, 3-fluoro-4-dodecyloxybenzoic acid chloride 3.32 and (S)-2-methylbutyl 4'-hydroxybiphenyl-4-carboxylate 2.84 g were reacted in pyridine 10 and CH2Cl2 15 mL for 3 h under reflux. After the reaction mixture cooled, Et acetate 50 mL was added and washing twice with 10% HCl and once each with saturated NaHCO3 aqueous solution and saturated NaCl aqueous solution were performed. After the reaction. product was dried with anhydrous Na sulfate, the solvent was concentrated The crude crystals obtained were purified by column chromatog. on SiO2 gel with CHCl3/hexane and recrystd. from EtOH to obtain 4.64 g of 4-(4-[(S)-2-methylbutyloxycarbonyl]phenyl)phenyl 3-fluoro-4-dodecyloxybenzoate (II). II was heated at 160° to form an isotropic liquid and placed in a thin cell. The cell was cooled at 5°/min to align the smectic phase and a uniform monodomain was obtained. The cell was cooled to <118° to obtain a chiral smectic C phase. An elec. field (20 V, 50 Hz rectangular wave] was applied at 102° and the light switching action took 100 μs. When a triangular wave was applied to the cell at 102° the spontaneous polarization was 2.24 nC/cm2.

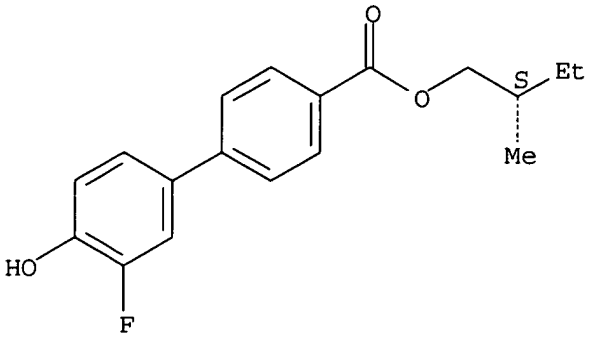
IT **106316-31-8P**

RL: PREP (Preparation)
(preparation of, for liquid-crystal display devices)

RN 106316-31-8 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 3'-fluoro-4'-hydroxy-, 2-methylbutyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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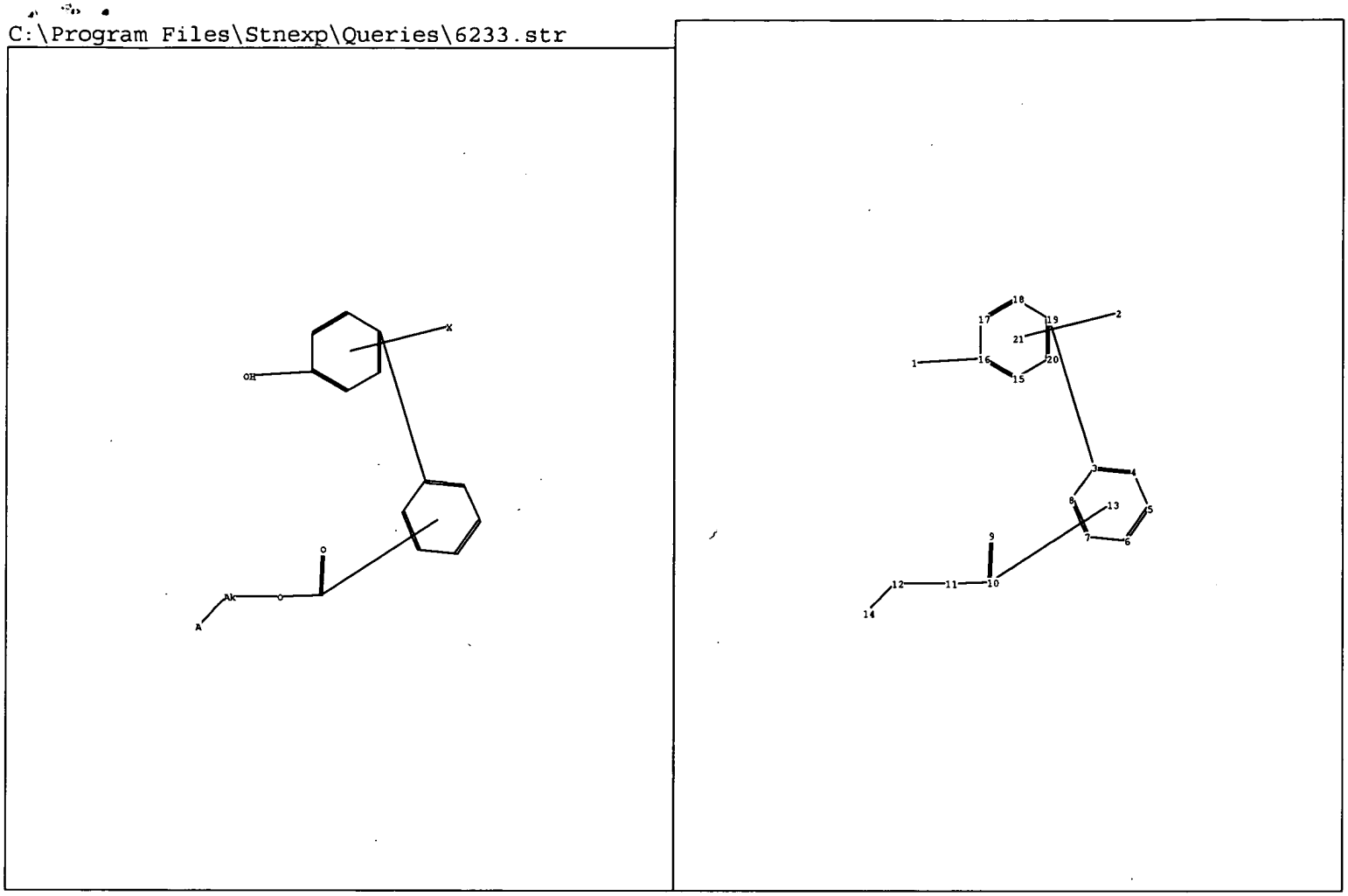

chain nodes :
1 2 9 10 11 12 14
ring nodes :
3 4 5 6 7 8 15 16 17 18 19 20
chain bonds :
1-16 3-19 9-10 10-11 11-12 12-14
ring bonds :
3-8 3-4 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds :
1-16 9-10 10-11 11-12 12-14
exact bonds :
3-19
normalized bonds :
3-8 3-4 4-5 5-6 6-7 7-8 15-16 15-20 16-17 17-18 18-19 19-20

Match level :
1:CLASS 2:CLASS 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:CLASS